

Methyl acetate
79-20-9 | DTXSID4021767

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.23e-01

Global applicability domain: Inside

Local applicability domain index: 6.51e-01

Confidence level: 6.63e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Methyl acetate</div> <div>Measured: 0.18</div> <div>Predicted: 1.23e-01</div>	<div>Image not found</div> <div>Ethyl formate</div> <div>Measured: 0.23</div> <div>Predicted: 2.38e-01</div>	<div>Image not found</div> <div>2-Fluoroethanol</div> <div>Measured: -0.670</div> <div>Predicted: -0.450</div>
<div>Image not found</div> <div>Methyl propanoate</div> <div>Measured: 0.84</div> <div>Predicted: 7.41e-01</div>	<div>Image not found</div> <div>2-Propanol, 1,3-difluoro-</div> <div>Measured: -0.360</div> <div>Predicted: -0.0748</div>	